Modelling and design of stress-induced martensite formation in metastable β Ti alloys

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ABSTRACT

The temperature dependence of the stress-induced martensite (SIM) formation in a Ti–10V–2Fe–3Al (Ti-1023) alloy under compressive loading has been studied. At low temperatures, the stress level at which martensite starts to form increases linearly with the deformation temperature, while the stress at which the deformation switches to regular plastic deformation is roughly temperature independent. A thermostatistical model for dislocation evolution is employed to describe deformation twinning in martensite. Combined effects of twinning induced plasticity and solid solution strengthening are considered in terms of temperature variations. The SIM effect disappears on deformation at temperatures beyond ~ 233 °C, which is close to the predicted M_s temperature of 240 °C. The thermostatistical model predicts a transition from twinned martensite to pure slip at 250 °C. By providing a model to predict the martensite formation, and by describing deformation twinning, the present work provides a number of tools that may be employed to conceive new titanium alloys combining improved strength and ductility.

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1. Introduction

Several challenges are faced by titanium alloys towards their commercialisation and widespread use. Although recent progress has been made in their cost reduction, issues such as strong texture and poor formability remain a challenge [1]. A way to increase formability is by exploitation of their ability to form martensite under stress around room temperature. Athermal martensite forms on quenching from a high temperature phase, inducing a phase transformation triggered by the co-ordinated production of stacking faults. This process has been described by Olson and Cohen for a variety of parent (high temperature phase) and product (martensite) crystal structures [2–4]. The product phase formed on quenching undergoes only *incomplete* transformation, as this is arrested by the adjoining high temperature phase, which becomes retained when quenching to room temperature. Further martensite formation becomes possible at low temperature by supplying an extra amount of

energy by mechanical means. This is referred to as *stress-induced martensite* (SIM), which deformation may lead to concomitant improvements in strength and ductility, as has been demonstrated in steel technology [5].

SIM formation is a widely observed phenomenon in β and near β titanium alloys [6–10]. A sufficiently high level of β stabilising elements the diffusional β (austenite) to α phase transformation, leading to a metastable β, which potentially can transform to martensite or ω phase [11–13]. The transformation from metastable β to martensite can occur either athermally or under the influence of stress, depending on alloy composition and deformation temperature, which eventually determines the SIM formation capability. Recent studies have shown that the SIM effect can be tailored to achieve improvements in the mechanical properties of the near β-Ti–10V–2Fe–3Al (Ti-1023) alloy [14]. The key factor which controls the deformation induced martensite formation at room temperature is the composition of the β (austenite) phase, which determines its metastability and M_s temperature. The composition of the β phase itself is defined by the heat treatment conditions. The range of heat treatment conditions leading to enhanced metastability of the β phase, required to trigger martensite formation upon deformation at room temperature, has been identified for the Ti-1023 alloy [14]. Such treatments resulted in an increase in the compressive strength by $\sim 20\%$ due to the presence of SIM [14]. However, little is known about the temperature dependence of the SIM phenomenon and its

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relation to the athermal M_s temperature. Additionally, by assuming that martensite plays a dominant role during work hardening, a thermodynamics-based deformation twinning model (for hexagonal metals) is employed to describe the experimental stress–strain curves. Central to this approach is the introduction of the statistical entropy accounting for the possible dislocation migration paths. This allows one to obtain an expression for the dislocation recovery term as a function of the energy barrier for dislocation annihilation [15]. Based on a Kocks–Mecking formulation, a dislocation density evolution equation has been derived to characterise solid solution effects. On the other hand, deformation twinning in pure hexagonal materials has been described by incorporating an additional dislocation generation term for twin propagation [16]. Such a term becomes active once a critical strain for twin nucleation is reached. The current work aims at describing, both experimentally and theoretically, the temperature dependence of the SIM properties in metastable β Ti-1023 alloy and the transition temperature from SIM deformation mode to regular plastic deformation via dislocation motion. The model combines multicomponent and deformation twinning effects for describing twinning deformation in martensite. The capacity to apply these concepts for the conception of titanium alloys of improved strength and ductility is discussed.

2. Thermostatistical model for plasticity

2.1. Energy barrier for dynamic recovery

The Kocks–Mecking equation [17] has recently been subjected to a thermodynamic analysis [15] aimed at obtaining expressions for the dynamic recovery rate f_{DRV}, in terms of an annihilating dislocation segment (of length l)

$$\frac{d\rho(\gamma)}{d\gamma} = \frac{d\rho^+}{d\gamma} - f_{DRV}\rho(\gamma), \tag{1}$$

where ρ is the average dislocation density, γ is the shear strain, and $d\rho^+/d\gamma$ is the dislocation generation rate (presented in the following sections). Such an analysis leads to an expression for f_{DRV} in terms of an energy barrier for dislocation annihilation $\langle \Delta G \rangle$ in multicomponent systems. $\langle \Delta G \rangle$ is composed of the addition of five terms [15]:

1. A dislocation formation energy term, approximated by the strain energy around the annihilating segment: $U_{form} = \frac{1}{2}\mu b^2 l$, where μ is the shear modulus and b is the magnitude of the Burgers vector.
2. A migration energy term: $U_{mig} = \sigma_Y A_{act} b^2 l$, where σ_Y is the yield stress and A_{act} is the (dimensionless) activation area for cross-slip.
3. A vacancy energy contribution to dislocation annihilation at higher temperatures (via dislocation climb), induced by the vacancy chemical work around the segment: $U_{vac} = (V_{sys}/b^3) \delta(E_f + k_B T \ln c_m)$, where $V_{sys} = l^* l b$ is the volume of the annihilating system (a dislocation distortion's field length on a slip plane), $l^* = 12.5b$ is the dislocation's distortion field length ($\sim$98% of the total strain field induced by the dislocation [18]); E_f is the vacancy formation energy, c_m is the vacancy concentration at the melting point (T_m), and $\delta(T)$ is a continuum piecewise function that vanishes the vacancy contribution ($\delta = 0$) at low temperatures[3] ($T < T_0$), increases linearly at medium temperatures ($T_0 < T < T_f$), and becomes fully present ($\delta = 1$) at high temperatures ($T > T_f$).
4. A dislocation-solute atom interaction energy term, approximated by the solute chemical potential around the segment:

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[3] Definitions of T_0 and T_f are presented in

$U_{SS} = V_{sys} \sum_i x_i \Delta G_{sys}$, where x_i is the atomic fraction of the i solute element, and ΔG_{sys} is the free energy of the mixture.

5. A statistical entropy contribution $T\Delta S$ accounting for the energy dissipation due to the energetically *favourable* dislocation paths active during deformation.

The addition of these terms leads to

$$\langle \Delta G \rangle = \frac{b}{l}(U_{form} + U_{mig} + U_{vac} + U_{SS} - T\Delta S), \tag{2}$$

where the factor b/l scales the energy contributions to the number of particles along the dislocation line participating in the annihilation process. In a thermally activated process, the expected velocity for a dislocation to undergo annihilation can be expressed in terms of an Arrhenius equation, where $\langle \Delta G \rangle$ is the energy to be overcome. Combining the previous expressions, l can be obtained. A detailed analysis on how to derive l can be found in [18].

2.2. Quantification of the number of microstates

Instead of trying to describe the instantaneous velocity gradient at every moment, the entropy accounts for the total energy loss due to the different dislocation velocity configurations. A microstate is defined as the number of interatomic subunits a dislocation segment can glide during an arbitrary time step Δt [18]. At high temperatures, vacancy–dislocation interactions become prominent, increasing dislocation motion events via vacancy-assisted climb and consequently additional number of microstates are incorporated [19]. The total number of microstates (dislocation slip+climb) Ω becomes [18,19]

$$\Omega = \Omega_{dis} + \Omega_{v-d} = \left(\frac{\dot{\varepsilon}_0 + \vartheta}{\dot{\varepsilon}}\right), \tag{3}$$

where Ω_{dis} and Ω_{v-d} are the number of microstates due to dislocation slip and to vacancy–dislocation interaction respectively, $\dot{\varepsilon}_0 = cb\rho_Y$ is a limiting value for strain rate, this is achieved when the dislocations approach the speed of sound in the material, c, ρ_Y is the dislocation density consistent with the yield point ($\rho_Y = (\sigma_Y/0.9\mu b)^2$ [18]), $\dot{\varepsilon}$ is the strain rate; $\vartheta = \vartheta_D \exp(-E_m/RT)$ is the vacancy migration frequency, wherein $\vartheta_D = 10^{13}$ s^{-1} is the Debye frequency, E_m is the vacancy migration energy, R is the gas constant and T is the absolute temperature.

2.3. Low and high temperature deformation regimes

The transition temperatures for different dislocation annihilation mechanisms are obtained by comparing Ω_{dis} and Ω_{v-d} [19]: $T_0 = E_m/R \ln(\vartheta_D/\dot{\varepsilon})$, when only one vacancy–dislocation interaction microstate is available; and $T_f = E_m/R \ln(\vartheta_D/\dot{\varepsilon}_0)$, when vacancy–dislocation microstates equal those for pure slip. Below T_0 no vacancy effect is present and cross-slip is the main annihilation mechanism; above T_f vacancy-assisted dislocation climb is the predominant annihilation mechanism; and between these values, both mechanisms take place. In pure FCC and HCP metals it has been found that $0.2T_m \leq T_0 \leq 0.3T_m$ and $0.5T_m \leq T_f \leq 0.6T_m$, these values being in good agreement with the transition ranges usually considered in the literature [16,19].

2.4. Entropy and dynamic recovery rate

The statistical entropy for pure metals equals [18]

$$\Delta S = k_B \ln \Omega = k_B \ln \left(\frac{\dot{\varepsilon}_0 + \vartheta}{\dot{\varepsilon}}\right). \tag{4}$$

The dynamic recovery term equals the fraction of the substance undergoing dislocation annihilation per dislocation and is